



# **STIC Search Report**

## **EIC 1700**

**STIC Database Tracking Number: 112822**

**TO: Dawn Garrett**  
**Location: REM 5C 75**  
**Art Unit : 1774**  
**January 30, 2004**

**Case Serial Number: 10/644872**

**From: Barba Koroma**  
**Location: EIC 1700**  
**REM EO4 A30**  
**Phone: 571 272 2546**

**barba.koroma@uspto.gov**

### **Search Notes**

Examiner Garrett,

Please find attached results of the search you requested. Various components of the claimed invention as spelt out in the claims were searched in REGISTRY and CAPLUS databases. For your convenience, titles of hits have been listed to help you peruse the results set quickly. This is followed by a detailed printout of records. Please let me know if you have any questions.

Thanks.

=> file reg

FILE 'REGISTRY' ENTERED AT 11:15:12 ON 30 JAN 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 28 JAN 2004 HIGHEST RN 642928-00-5  
DICTIONARY FILE UPDATES: 28 JAN 2004 HIGHEST RN 642928-00-5

TSKA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> file caplus

FILE 'CAPLUS' ENTERED AT 11:15:17 ON 30 JAN 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

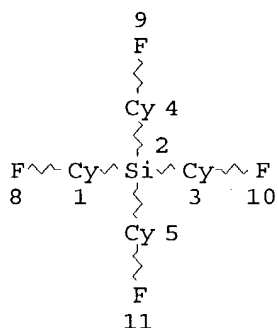
Copyright of the articles to which records in this database refer is  
held by the publishers listed in the PUBLISHER (PB) field (available  
for records published or updated in Chemical Abstracts after December  
26, 1996), unless otherwise indicated in the original publications.  
The CA Lexicon is the copyrighted intellectual property of the  
American Chemical Society and is provided to assist you in searching  
databases on STN. Any dissemination, distribution, copying, or storing  
of this information, without the prior written consent of CAS, is  
strictly prohibited.

FILE COVERS 1907 - 30 Jan 2004 VOL 140 ISS 6  
FILE LAST UPDATED: 29 Jan 2004 (20040129/ED)

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

=> d que

L57 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L58 ( 6)SEA FILE=REGISTRY SSS FUL L57

L59 20 SEA FILE=CAPLUS ABB=ON PLU=ON L58

=> d ti 1-20

L59 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

TI Intramolecular interactions in aromatic compounds: V. Electronic structure of polyfluoroaromatic silanes and related hydrocarbons

L59 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

TI Olefin polymerization and process therefor

L59 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

TI Substituent effect on electronegativity of Ar<sub>3</sub>Si and Ar<sub>3</sub>Sn groups: comparison of the results of ab initio quantum-chemical calculations with 19F NMR data for Ar<sub>3</sub>MQC<sub>6</sub>H<sub>4</sub>F-4 compounds

L59 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

TI A convenient preparation of pentafluorophenyl(fluoro)silanes: reactivity of pentafluorophenyltrifluorosilane

L59 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

TI Thermodynamic simulation of deposition of molybdenum and tungsten disilicides in metalorganic CVD processes

L59 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

TI Photoelectron helium spectra of the pentafluorophenyl derivatives of Group IV and V elements

- L59 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Reactions of arylmethyilsilanes and tetraarylsilanes with xenon difluoride in the presence of fluoride ions
- L59 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Pentafluorophenyliodine(V) compounds, part 1. Preparation of pentafluorophenyliodine tetrafluoride and other aryliodine tetrafluorides by reaction of iodine pentafluoride with arylsilanes
- L59 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI The crystal structure of tetrakis(pentafluorophenyl)silane
- L59 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI A fluorine-19 NMR investigation of the transmission of electronic effects in triaryl(4-fluorophenyl)silanes
- L59 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI NMR studies of pentafluorophenyl-substituted silanes. I. Relations between chemical shifts, coupling constants, and (p-d) $\pi$  interactions
- L59 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Fragmentation and rearrangement processes in the mass spectra of perhalogenoaromatic compounds. II. Pentafluorophenyl derivatives of group IV
- L59 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI A direct preparation of some pentafluorophenyl-containing silanes
- L59 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI The fluorine-19 NMR spectra of some pentafluorophenyl compounds of group IV elements
- L59 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Polyhalo-organometallic and -organometalloidal compounds. VIII. Preparation of some pentafluorophenyl substituted organosilicon compounds
- L59 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Pentafluorophenyl organometallic compounds of group IV elements
- L59 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Tetrakis(pentafluorophenyl)silane
- L59 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Pentafluoriodobenzene
- L59 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Synthesis of organosilicon compounds, particularly those containing halophenyl groups
- L59 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Preparation and thermal stability of tetrakis(pentafluorophenyl)silane and

tris(pentafluorophenyl)phosphine

=> d ibib abs hitstr ind total

L59 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:525583 CAPLUS

DOCUMENT NUMBER: 133:252494

TITLE: Intramolecular interactions in aromatic compounds: V.  
Electronic structure of polyfluoroaromatic silanes and  
related hydrocarbons

AUTHOR(S): Krupoder, S. A.; Okotrub, A. V.; Villem, N. V.;  
Villem, J. J.; Furin, G. G.; Salakhutdinov, N. F.;  
Poleshchuk, O. Kh.

CORPORATE SOURCE: Institute of Organic Chemistry, Siberian Branch,  
Russian Academy of Sciences, Novosibirsk, Russia

SOURCE: Russian Journal of General Chemistry (Translation of  
Zhurnal Obshchei Khimii) (2000), 70(1), 101-110  
CODEN: RJGCEK; ISSN: 1070-3632

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The electronic structure of pentafluorophenyl-substituted silanes  
Ar<sub>n</sub>SiMe<sub>4-n</sub> (Ar = C<sub>6</sub>H<sub>5</sub>, C<sub>6</sub>F<sub>5</sub>, 4-FC<sub>6</sub>H<sub>4</sub>, 2,3,5,6-F<sub>4</sub>C<sub>5</sub>N; n = 1; Ar = C<sub>6</sub>H<sub>5</sub>,  
C<sub>6</sub>F<sub>5</sub>, n = 2, 4) was studied by x-ray emission and He(I) photoelectron  
spectroscopy. The He(I) photoelectron spectra were measured and  
interpreted from MNDO calcns., anal. of the p-fluoro effect, and relative  
intensities. Substitution of C<sub>6</sub>F<sub>5</sub> for C<sub>6</sub>H<sub>5</sub> in aryltrimethyl- and  
diaryldimethylsilanes results in enhanced  $\pi$  interaction between the  
aryl and SiMe<sub>n</sub> groups (n = 2, 3) by higher  $\pi$  levels and has almost no  
effect on the charge on the Si atom.

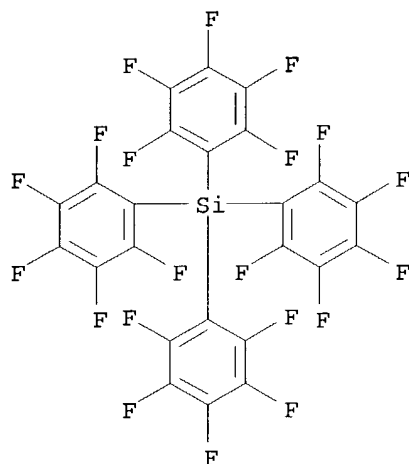
IT 1524-78-3, Tetrakis(pentafluorophenyl)silane

RL: PRP (Properties)

(electronic structure determined by photoelectron spectra, x-ray emission  
and MNDO calcns.)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



- CC 29-6 (Organometallic and Organometalloidal Compounds)  
Section cross-reference(s): 22
- ST electronic structure silane phenyl fluorophenyl MNDO; photoelectron spectrum silane phenyl fluorophenyl; x ray emission silane phenyl fluorophenyl; fluorine substituent effect photoelectron spectrum fluorophenylsilane
- IT Electronic structure  
MNDO (molecular orbital)  
Photoelectron spectra  
X-ray emission  
(of Ph and polyfluoroarom. silanes)
- IT Substituent effects  
(of fluorine in polyfluoroarom. silanes on photoelectron spectra)
- IT Ionization potential  
(of polyfluoroarom. silanes)
- IT Silanes  
RL: PRP (Properties)  
(polyfluoroarom.; electronic structure determined by photoelectron spectra, x-ray emission and MNDO calcns.)
- IT 455-17-4, 4-Fluorophenyl(trimethyl)silane 768-32-1,  
Trimethyl(phenyl)silane 778-24-5, Dimethyl(diphenyl)silane 1048-08-4,  
Tetraphenylsilane 1206-46-8, Pentafluorophenyl(trimethyl)silane  
**1524-78-3**, Tetrakis(pentafluorophenyl)silane 10536-62-6  
16297-29-3  
RL: PRP (Properties)  
(electronic structure determined by photoelectron spectra, x-ray emission and MNDO calcns.)
- IT 75-76-3, Tetramethylsilane  
RL: PRP (Properties)  
(model compound; electronic structure determined by photoelectron spectra, x-ray emission and MNDO calcns.)
- REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L59 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:490675 CAPLUS  
 DOCUMENT NUMBER: 129:149360  
 TITLE: Olefin polymerization and process therefor  
 INVENTOR(S): Van Tol, Maurits Frederik Hendrik  
 PATENT ASSIGNEE(S): DSM N.V., Neth.; Van Tol, Maurits Frederik Hendrik  
 SOURCE: PCT Int. Appl., 21 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9830603	A1	19980716	WO 1997-NL696	19971215
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
NL 1004991	C2	19980715	NL 1997-1004991	19970114
AU 9853475	A1	19980803	AU 1998-53475	19971215
EP 954540	A1	19991110	EP 1997-950491	19971215
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE, PT, FI				
CN 1248979	A	20000329	CN 1997-182023	19971215
JP 2002514247	T2	20020514	JP 1998-530771	19971215
US 6218487	B1	20010417	US 1999-352842	19990713
PRIORITY APPLN. INFO.:			NL 1997-1004991	A 19970114
			US 1997-38160P	P 19970213
			WO 1997-NL696	W 19971215

OTHER SOURCE(S): MARPAT 129:149360

AB Olefins are polymerized by contact with a transition metal catalyst, wherein the cocatalyst is either XR<sub>4</sub> (X = Si, Ge, Sn, Pb; R = H, alkyl, aryl, arylalkyl, alkylaryl; at least one R is not H and contains one or more halogen atoms) or is [X'R'<sub>5</sub>]-Y<sup>+</sup> (X' = Si, Ge, Sn, Pb; R' = H, alkyl, aryl, arylalkyl, alkylaryl; at least one R is not hydrogen and contains one or more halogen atoms; Y<sup>+</sup> = cation); the cocatalyst replaces aluminoxanes which can be difficult to remove from polyolefin products. Thus, [(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>SiMe]-[Li(THF)<sub>4</sub>]<sup>+</sup> was prepared and used with bis(cyclopentadienyl)zirconium monohydride monochloride and trioctylaluminum to polymerize ethylene.

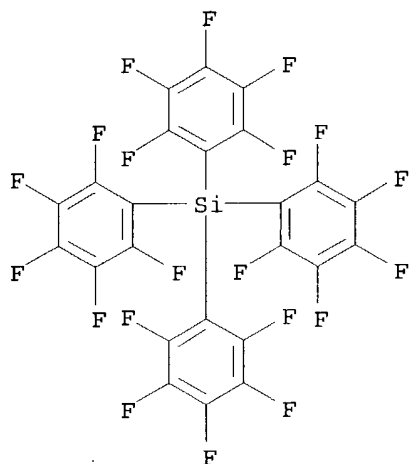
IT 1524-78-3P, Tetrakis(pentafluorophenyl)silane

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(cocatalyst intermediate; organosilane cocatalysts for polymerization of ethylene)

RN 1524-78-3 CAPLUS

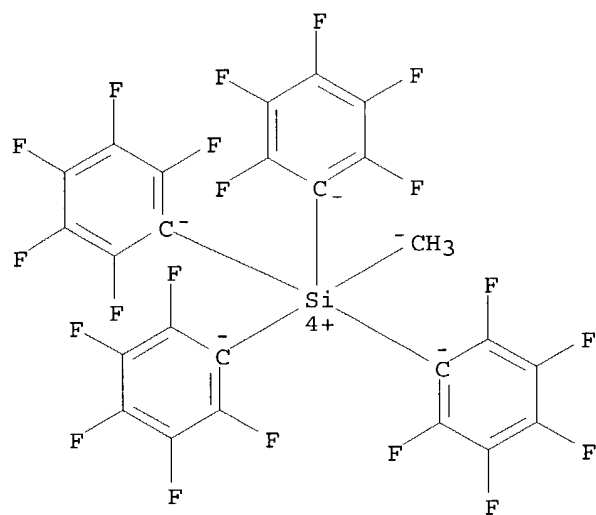
CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 210771-45-2DP, reaction products with triphenylchloromethane  
 210771-45-2P  
 RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);  
 USES (Uses)  
 (cocatalyst; organosilane cocatalysts for polymerization of ethylene)  
 RN 210771-45-2 CAPLUS  
 CN Lithium(1+), tetrakis(tetrahydrofuran)-, (T-4)-,  
 methyltetrakis(pentafluorophenyl)silicate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 210771-44-1  
 CMF C25 H3 F20 Si  
 CCI CCS



KOROMA EIC1700

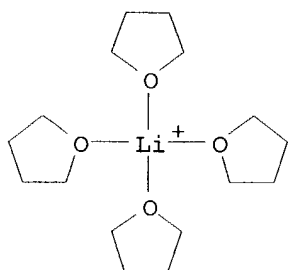


CM 2

CRN 48186-27-2

CMF C16 H32 Li O4

CCI CCS



RN 210771-45-2 CAPLUS

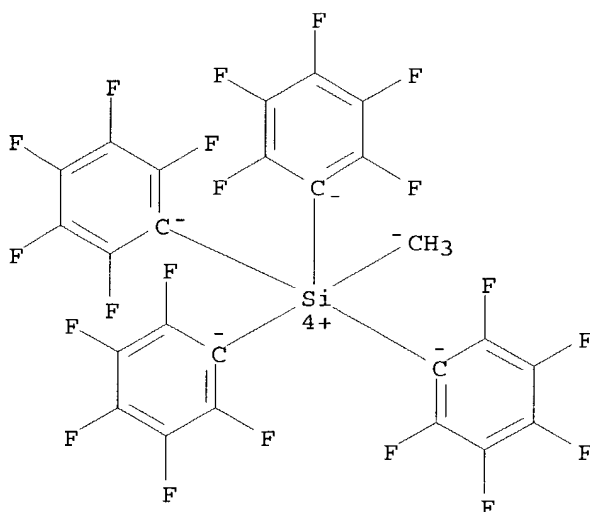
CN Lithium(1+), tetrakis(tetrahydrofuran)-, (T-4)-, methyltetrakis(pentafluorophenyl)silicate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 210771-44-1

CMF C25 H3 F20 Si

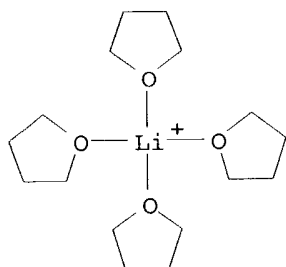
CCI CCS



CM 2

KOROMA EIC1700

CRN 48186-27-2  
CMF C16 H32 Li O4  
CCI CCS



IC ICM C08F004-60  
ICS C08F010-00; C07F007-08  
CC 35-3 (Chemistry of Synthetic High Polymers)  
ST ethylene polymn catalyst organosilane organozirconium; polyolefin prodn  
catalyst silicon germanium  
IT Polymerization catalysts  
(metallocene; organosilane and -germane cocatalysts for polymerization of  
olefins)  
IT Polymerization catalysts  
(organosilane and -germane catalysts for polymerization of olefins)  
IT Polyolefins  
RL: IMF (Industrial manufacture); PREP (Preparation)  
(organosilane and -germane cocatalysts for polymerization of olefins)  
IT 67108-80-9, Bis(pentamethylcyclopentadienyl)dimethylzirconium  
RL: CAT (Catalyst use); USES (Uses)  
(catalyst; organogermanium cocatalysts for polymerization of ethylene)  
IT 1070-00-4, Trioctylaluminum 37342-97-5 178762-91-9 210771-60-1  
RL: CAT (Catalyst use); USES (Uses)  
(catalyst; organosilane cocatalysts for polymerization of ethylene)  
IT 5121-90-4P  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
(Reactant or reagent)  
(cocatalyst intermediate; organosilane and -germane cocatalysts for  
polymerization of ethylene)  
IT 1524-78-3P, Tetrakis(pentafluorophenyl)silane  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
(Reactant or reagent)  
(cocatalyst intermediate; organosilane cocatalysts for polymerization of  
ethylene)  
IT 10038-98-9P, Tetrachlorogermane  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
(Reactant or reagent)  
(cocatalyst starting material; organogermanium cocatalysts for  
polymerization  
of ethylene)

KOROMA EIC1700

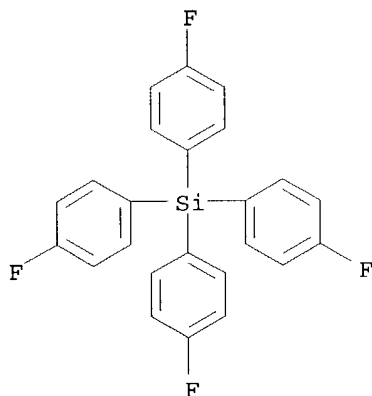
- IT 917-54-4, Methyllithium 1074-91-5, 1-Bromo-2,3,4,5-tetrafluorobenzene  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cocatalyst starting material; organosilane and -germane cocatalysts for polymerization of ethylene)
- IT 344-04-7, Pentafluorobromobenzene 10026-04-7, Tetrachlorosilane  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cocatalyst starting material; organosilane cocatalysts for polymerization of ethylene)
- IT 13628-95-0P  
 RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)  
 (cocatalyst; organogermanium cocatalysts for polymerization of ethylene)
- IT 1452-12-6P, Tetrakis(pentafluorophenyl)germane  
 RL: CAT (Catalyst use); IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (cocatalyst; organogermanium cocatalysts for polymerization of ethylene)
- IT 210771-66-7DP, reaction products with triphenylchloromethane 210771-66-7P  
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
 (cocatalyst; organogermanium cocatalysts for polymerization of ethylene)
- IT 210771-45-2DP, reaction products with triphenylchloromethane 210771-45-2P 210771-81-6P  
 RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)  
 (cocatalyst; organosilane cocatalysts for polymerization of ethylene)
- IT 52910-17-5P  
 RL: CAT (Catalyst use); IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (cocatalyst; organosilane cocatalysts for polymerization of ethylene)
- IT 76-83-5DP, Triphenylchloromethane, reaction products with organosilanes and organogermanes  
 RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)  
 (cocatalysts; organosilane and -germane cocatalysts for polymerization of ethylene)
- IT 210771-81-6DP, reaction products with triphenylchloromethane  
 RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)  
 (cocatalysts; organosilane cocatalysts for polymerization of ethylene)
- IT 925-90-6, Ethylmagnesium bromide  
 RL: NUU (Other use, unclassified); USES (Uses)  
 (in preparation of organosilane cocatalysts for polymerization of ethylene)
- IT 9002-88-4P  
 RL: IMF (Industrial manufacture); PREP (Preparation)  
 (organosilane and -germane cocatalysts for polymerization of ethylene)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

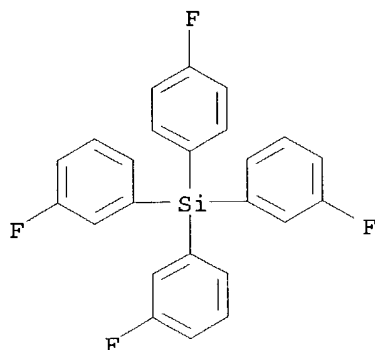
L59 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1996:120497 CAPLUS

KOROMA EIC1700

DOCUMENT NUMBER: 124:261208  
 TITLE: Substituent effect on electronegativity of Ar<sub>3</sub>Si and Ar<sub>3</sub>Sn groups: comparison of the results of ab initio quantum-chemical calculations with <sup>19</sup>F NMR data for Ar<sub>3</sub>MQC<sub>6</sub>H<sub>4</sub>F-4 compounds  
 AUTHOR(S): Kravtsov, D. N.; Peregodov, A. S.; Shcherbakova, O. V.; Borisov, Yu. A.  
 CORPORATE SOURCE: A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, 117813, Russia  
 SOURCE: Izvestiya Akademii Nauk, Seriya Khimicheskaya (1995), (10), 1921-4  
 CODEN: IASKEA  
 PUBLISHER: Institut Organicheskoi Khimii im. N. D. Zelinskogo Rossiiskoi Akademii Nauk  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB Ab initio calcns. for the group electronegativity  $\chi$  of Ar<sub>3</sub>Si and Ar<sub>3</sub>Sn groups containing 13 types of m-, p- and polysubstituted Ph groups was performed. The calculated values of  $\chi$ (Ar<sub>3</sub>Si) and  $\chi$ (Ar<sub>3</sub>Sn) correlate better with the  $\sigma_0$  Taft consts. then with  $\sigma$  Hammett consts., which provides evidence for the inductive effect of aryl groups. Good correlation was found for <sup>19</sup>F chemical shifts in Ar<sub>3</sub>SiC<sub>6</sub>H<sub>4</sub>F-4, Ar<sub>3</sub>SnC<sub>6</sub>H<sub>4</sub>F-4, Ar<sub>3</sub>SnCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>F-4 and Ar<sub>3</sub>SnSC<sub>6</sub>H<sub>4</sub>F-4 with the corresponding values of  $\chi$ (Ar<sub>3</sub>Si) and  $\chi$ (Ar<sub>3</sub>Sn).  
 IT 63523-07-9 175029-06-8  
 RL: PRP (Properties)  
 (substituent effect on electronegativity of triarylsilyl and triarylstannyl groups in substituted fluorobenzenes)  
 RN 63523-07-9 CAPLUS  
 CN Silane, tetrakis(4-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 175029-06-8 CAPLUS  
 CN Silane, tris(3-fluorophenyl)(4-fluorophenyl)- (9CI) (CA INDEX NAME)



CC 29-8 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 22

ST group electronegativity silyl stannyl substituent effect; triarylsilyl  
 group electronegativity substituent effect; triarylstannyl group  
 electronegativity substituent effect; Taft substituent const  
 triarylstannyl triarylsilyl group

IT Electronegativity  
 Linear free energy relationship  
 Substituent effect  
 (substituent effect on electronegativity of triarylsilyl and  
 triarylstannyl groups)

IT Molecular orbital  
 (MNDO, of triarylstannyl- and triarylsilyl-substituted fluorobenzenes)

IT Substituent constant  
 (Taft, substituent effect on electronegativity of triarylsilyl and  
 triarylstannyl groups)

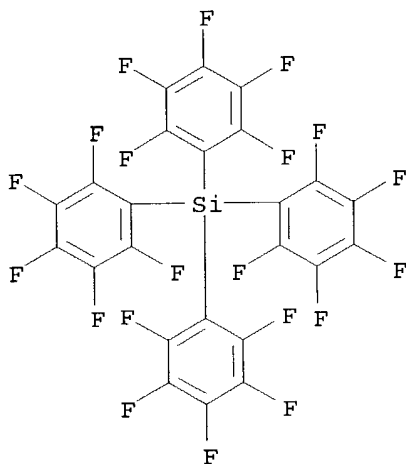
IT Functional groups  
 (silyl, triarylsilyl; substituent effect on electronegativity of  
 triarylsilyl and triarylstannyl groups)

IT Functional groups  
 (stannyl, triarylstannyl; substituent effect on electronegativity of  
 triarylsilyl and triarylstannyl groups)

IT 426-81-3 1251-03-2 34243-46-4 38186-04-8 51053-80-6 51053-81-7  
 51053-82-8 51053-83-9 51107-58-5 51107-59-6 51107-60-9  
 51107-61-0 51107-62-1 51107-63-2 63523-02-4 63523-03-5  
 63523-04-6 63523-05-7 63523-06-8 **63523-07-9** 63523-08-0  
 63523-09-1 63523-11-5 78788-05-3 78788-06-4 78788-07-5  
 78788-08-6 78788-09-7 78788-10-0 78788-11-1 78788-12-2  
 78795-74-1 84761-46-6 84761-47-7 84761-48-8 84761-49-9  
 84761-50-2 84761-51-3 84761-52-4 84761-53-5 84761-54-6  
**175029-06-8** 175029-07-9  
 RL: PRP (Properties)  
 (substituent effect on electronegativity of triarylsilyl and  
 triarylstannyl groups in substituted fluorobenzenes)

L59 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1996:58862 CAPLUS

DOCUMENT NUMBER: 124:232542  
 TITLE: A convenient preparation of  
 pentafluorophenyl(fluoro)silanes: reactivity of  
 pentafluorophenyltrifluorosilane  
 AUTHOR(S): Frohn, H. J.; Giesen, M.; Klose, A.; Lewin, A.;  
 Bardin, V. V.  
 CORPORATE SOURCE: Fachgebiet Anorganische Chemie, Gerhard-Mercator-  
 Universitaet Duisburg, Lotharstr. 1, Duisburg,  
 D-47048, Germany  
 SOURCE: Journal of Organometallic Chemistry (1996), 506(1-2),  
 155-64  
 CODEN: JORCAI; ISSN: 0022-328X  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 124:232542  
 AB Pentafluorophenyl(fluoro)silanes (C<sub>6</sub>F<sub>5</sub>)<sub>n</sub>SiF<sub>4-n</sub> (n = 1, 2) were prepared from  
 the corresponding ethoxysilanes by sequential chlorodeethoxylation with  
 SOCl<sub>2</sub> and fluoridation of chlorosilanes with SbF<sub>3</sub>. The conversion of  
 C<sub>6</sub>F<sub>5</sub>Si(OEt)<sub>3</sub> and C<sub>6</sub>F<sub>5</sub>SiCl<sub>3</sub> into C<sub>6</sub>F<sub>5</sub>SiF<sub>3</sub> with anhydrous HF is described.  
 Some reactions of C<sub>6</sub>F<sub>5</sub>SiF<sub>3</sub> with electrophiles and nucleophiles were  
 studied.  
 IT 1524-78-3, Tetrakis(pentafluorophenyl)silane  
 RL: PRP (Properties)  
 (NMR)  
 RN 1524-78-3 CAPLUS  
 CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)  
 ST pentafluorophenylfluorosilane prepn reaction; silane  
 pentafluorophenylfluoro prepn reaction; ethoxysilane chlorodeethoxylation  
 fluoridation  
 IT Fluorination  
 (of pentafluorophenyl(chloro)silanes)

- IT Silanes  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(pentafluorophenyl(fluoro)silanes; preparation and reactions with electrophiles and nucleophiles)
- IT Ethoxylation  
(retro, chloro-; of pentafluorophenyl(ethoxy)silanes)
- IT 1524-78-3, Tetrakis(pentafluorophenyl)silane 20160-39-8,  
Chlorotris(pentafluorophenyl)silane 35370-01-5,  
Fluorotris(pentafluorophenyl)silane  
RL: PRP (Properties)  
(NMR)
- IT 371-20-0P, Diethoxy(fluoro)borane 86802-17-7P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(formation from pentafluorophenyltriethoxysilane and boron fluoride etherate)
- IT 344-04-7P, Bromopentafluorobenzene 174743-13-6P,  
Bromodifluoro(pentafluorophenyl)silane  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(formation from pentafluorophenyltrifluorosilane and bromine)
- IT 14188-35-3P, Dibromodifluorosilane 18356-67-7P, Tribromo(fluoro)silane  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(formation from pentafluorophenyltrifluorosilane and bromine/aluminum bromide)
- IT 7783-61-1P, Silicon tetrafluoride 121827-61-0P,  
Bis(pentafluorophenyl)iodonium  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(formation from pentafluorophenyltrifluorosilane and fluoroiodonium fluoroantimonate)
- IT 20160-47-8P, Chloro(ethoxy)bis(pentafluorophenyl)silane 174743-04-5P,  
Ethoxydifluoro(pentafluorophenyl)silane 174743-05-6P,  
Diethoxy(fluoro)(pentafluorophenyl)silane 174743-08-9P,  
Dichloro(ethoxy)(pentafluorophenyl)silane  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; convenient preparation of fluorophenyl(fluoro)silanes: reactivity of fluorophenylfluorosilane)
- IT 174743-11-4P, Dibutyl(ethoxy)(pentafluorophenyl)silane  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with acetyl chloride/zinc chloride)
- IT 20083-38-9P, Trichloro(pentafluorophenyl)silane 20160-45-6P,  
Dichlorobis(pentafluorophenyl)silane  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with antimony fluoride)
- IT 5272-26-4P, Trifluoro(pentafluorophenyl)silane  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reactions with electrophiles and nucleophiles)
- IT 27585-17-7P, Difluorobis(pentafluorophenyl)silane  
RL: SPN (Synthetic preparation); PREP (Preparation)

- (preparation and reactions with electrophiles and nucleophiles)
- IT 174743-06-7P, Difluoro(pentafluorophenyl) (1-piperidino)silane  
 174743-07-8P, Fluoro(pentafluorophenyl)bis(1-piperidino)silane  
 174743-09-0P, Tributyl(pentafluorophenyl)silane 174743-10-3P,  
 Dibutyl(fluoro)(pentafluorophenyl)silane 174743-12-5P,  
 Dibutyl(4-butyltetrafluorophenyl)(pentafluorophenyl)silane  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)
- IT 693-03-8, Bromo(butyl)magnesium  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with pentafluorophenyltrifluorosilane)
- IT 13888-69-2, Diethoxybis(pentafluorophenyl)silane  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with thionyl chloride/pyridinium chloride)
- IT 20083-34-5, Triethoxy(pentafluorophenyl)silane  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactions with hydrofluoric acid, thionyl chloride/pyridinium  
 chloride, boron fluoride and other reagents)
- IT 109-72-8, Butyllithium, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactions with pentafluorophenyltrifluorosilane)

L59 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:602108 CAPLUS

DOCUMENT NUMBER: 117:202108

TITLE: Thermodynamic simulation of deposition of molybdenum  
 and tungsten disilicides in metalorganic CVD processes

AUTHOR(S): Kuznetsov, F. A.; Titov, V. A.; Golubenko, A. N.;  
 Titov, A. A.

CORPORATE SOURCE: Inst. Inorg. Chem., Novosibirsk, 630090, USSR

SOURCE: Proceedings of SPIE-The International Society for  
 Optical Engineering (1992), 1783(Int. Conf.

Microelectron., 1992), 541-50

CODEN: PSISDG; ISSN: 0277-786X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Modeling of disilicide deposition in the systems with volatile metalorg.  
 and fluorinated Si organic compds. was performed for a number of systems  
 M-Si-C-H-Ar, M-Si-C-O-Cl-H-Ar, M-Si-C-H-F-Ar, M-Si-C-O-F-H-Ar (M = W, Mo).  
 In some of these systems (especially with fluorinated compds.) there are wider  
 regions of quasi-equilibrium deposition of disilicides.

IT 1524-78-3

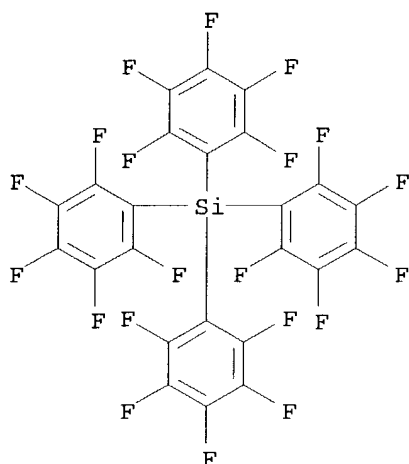
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with tungsten cyclopentadienyl complex in tungsten  
 disilicide deposition)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)





CC 75-1 (Crystallography and Liquid Crystals)  
 Section cross-reference(s): 69  
 ST deposition molybdenum tungsten silicide metalorg simulation  
 IT Vapor deposition processes  
 (of molybdenum and tungsten disilicide, thermodyn. simulation of  
 metalorg.)  
 IT 12039-88-2, Tungsten silicide (WSi<sub>2</sub>) 12136-78-6, Molybdenum silicide  
 (MoSi<sub>2</sub>)  
 RL: PEP (Physical, engineering or chemical process); PROC (Process)  
 (deposition of, thermodyn. simulation of metalorg. vapor-phase)  
 IT 1271-33-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with silicon compds. in tungsten disilicide deposition)  
 IT 1524-78-3 122571-42-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with tungsten cyclopentadienyl complex in tungsten  
 disilicide deposition)

L59 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:539948 CAPLUS

DOCUMENT NUMBER: 117:139948

TITLE: Photoelectron helium spectra of the pentafluorophenyl  
 derivatives of Group IV and V elements

AUTHOR(S): Petrachenko, N. E.; Vovna, V. I.; Furin, G. G.

CORPORATE SOURCE: Nauchno-Issled. Fiz.-Tekh.-Inst., Vladivostok, Russia

SOURCE: Zhurnal Fizicheskoi Khimii (1992), 66(2), 515-20

CODEN: ZFKHA9; ISSN: 0044-4537

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB In the compds. of tricoordinated P and As, intramol. interaction is observed  
 of a lone electron pair with the  $\pi$ -MO fluorinated benzene ring, while  
 in the P-containing compds. this interaction is stronger, than in As-containing  
 compds. In tetracoordinated compds., the interaction between orbitals of  
 the group X = O (X=P,As) with groups of  $\pi$ -MO substituents was not observed

The basic contribution to the bonding is from  $\sigma$ -orbitals localized on X-C bonds.

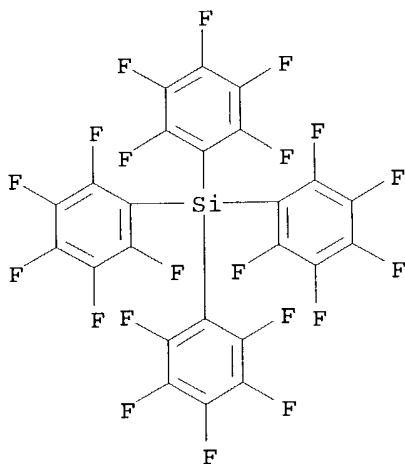
IT 1524-78-3

RL: PRP (Properties)

(photoelectron spectrum of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 73-6 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

ST photoelectron fluorophenyl Group IVA VA deriv; phenyl fluoro Group IVA VA photoelectron; bonding fluorophenyl Group IVA VA deriv

IT Bond

(in fluorophenyl derivs. of Group IVA and VA elements)

IT Photoelectron spectroscopy

(of pentafluorophenyl derivs. of Group IVA and VA elements)

IT 1065-49-2 1259-34-3 1259-35-4, Tris(pentafluorophenyl)phosphine  
1452-12-6 1524-78-3 2729-11-5, Tris(pentafluorophenyl)phosphine  
oxide 18005-77-1

RL: PRP (Properties)

(photoelectron spectrum of)

L59 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:534254 CAPLUS

DOCUMENT NUMBER: 111:134254

TITLE: Reactions of arylmethylsilanes and tetraarylsilanes with xenon difluoride in the presence of fluoride ions

AUTHOR(S): Bardin, V. V.; Stennikova, I. V.; Furin, G. G.;  
Leshina, T. V.; Yakobson, G. G.

CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR

SOURCE: Zhurnal Obshchei Khimii (1988), 58(11), 2580-8

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 111:134254

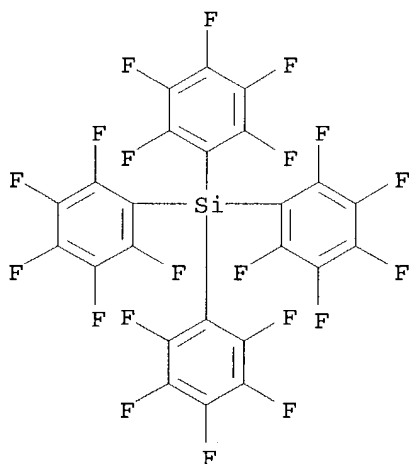
AB The reaction of  $RnSiMe_{4-n}$  ( $R = C_6F_5$ ,  $p-F_3CC_6F_4$ , tetrafluoro-4-pyridyl;  $n = 1, 2, 4$ ) with  $XeF_2$  in the presence of MF ( $M = K, Rb, Cs$ ) gave protodesilylation products and diaryls. The reaction is a convenient method for generation of polyfluoroaryl and polyfluorohetaryl radicals under mild conditions.

IT 1524-78-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with xenon difluoride)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 25, 27

ST arylmethylsilane xenon difluoride reaction; pyridylmethylsilane xenon difluoride reaction; xenon difluoride fluoroarylmethylsilane reaction; protodesilylation arylmethylsilane xenon difluoride reaction; radical polyfluoroaryl polyfluorohetaryl

IT Heterocyclic compounds

RL: PROC (Process)

(aromatic, fluoro, radicals, generation of, from reaction of  
hetarylmethylsilanes with xenon difluoride)

IT Aromatic hydrocarbons, preparation

RL: PREP (Preparation)

(fluoro, radicals, generation of, from reaction of arylmethylsilanes  
with xenon difluoride)

IT Silylation

(retro, in reaction of arylmethylsilanes with xenon difluoride)

IT 768-32-1, Trimethylphenylsilane 1048-08-4, Tetraphenylsilane  
3728-43-6, Trimethyl-p-tolylsilane 4405-33-8, Trimethyl-p-  
nitrophenylsilane

RL: RCT (Reactant); RACT (Reactant or reagent)

(attempted reaction of, with xenon difluoride)

IT 92-52-4P, 1,1'-Biphenyl, preparation 98-08-8P 344-04-7P 363-72-4P

434-90-2P 581-80-6P 651-80-9P 2875-18-5P 2875-19-6P 3511-91-9P  
 17823-47-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 IT 7789-23-3, Potassium fluoride 13400-13-0, Cesium fluoride 13446-74-7,  
 Rubidium fluoride  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of arylmethylsilanes with xenon difluoride in presence of)  
 IT 13709-36-9, Xenon difluoride  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with arylmethylsilanes)  
 IT 75-25-2, Tribromomethane  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with trimethylpentafluorophenylsilane and xenon  
 difluoride)  
 IT 312-75-4 1206-46-8 1524-78-3 16297-29-3 122571-41-9  
 122571-42-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with xenon difluoride)

L59 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1984:510434 CAPLUS

DOCUMENT NUMBER: 101:110434

TITLE: Pentafluorophenyl iodine(V) compounds, part 1.  
 Preparation of pentafluorophenyl iodine tetrafluoride  
 and other aryl iodine tetrafluorides by reaction of  
 iodine pentafluoride with arylsilanes

AUTHOR(S): Frohn, Hermann Josef

CORPORATE SOURCE: Fachber.-Chem., Univ. Gesamthochsch. Duisburg,  
 Duisburg, 4100/1, Fed. Rep. Ger.

SOURCE: Chemiker-Zeitung (1984), 108(4), 146-7  
 CODEN: CMKZAT; ISSN: 0009-2894

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 101:110434

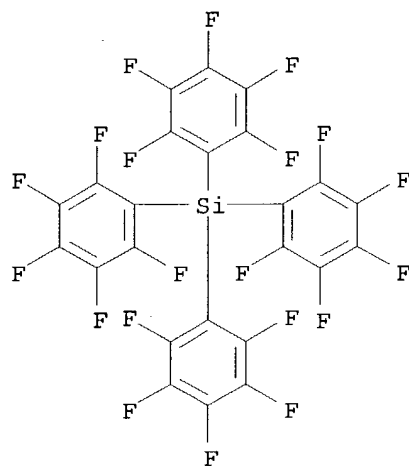
AB RIF4 (R = C6F5, Ph, p-F, -Me-, -MeOC6H4) were prepared by treating IF5 with  
 RnSiX4-n (X = F, Me; n = 1-4). The effect of solvent and pyridine on the  
 reaction was studied.

IT 1524-78-3 63523-07-9

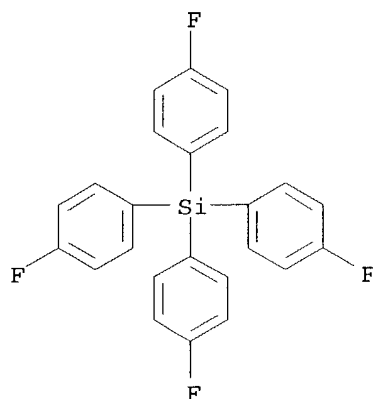
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with iodine pentafluoride)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 63523-07-9 CAPLUS  
 CN Silane, tetrakis(4-fluorophenyl)- (9CI) (CA INDEX NAME)



CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 29  
 ST fluorophenyl iodine tetrafluoride; phenyl iodine tetrafluoride; iodine  
 pentafluorophenyl tetrafluoride; silane phenyl iodine pentafluoride  
 reaction  
 IT Solvent effect  
 (on reaction of iodine pentafluoride with phenylsilanes)  
 IT 22121-26-2P 22121-27-3P 29848-54-2P 38091-68-8P 91679-75-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 IT 110-86-1, uses and miscellaneous  
 RL: USES (Uses)  
 (reaction of iodine pentafluoride with phenylsilanes in presence of)  
 IT 368-47-8 1048-08-4 1206-46-8 1524-78-3 5272-26-4  
 10256-83-4 10536-62-6 13688-78-3 24727-90-0 35370-01-5

KOROMA EIC1700

50625-30-4 63523-07-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with iodine pentafluoride)

IT 7783-66-6

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phenylsilanes)

IT 75-05-8, uses and miscellaneous

RL: PRP (Properties)  
(solvent effect of, on reaction of iodine pentafluoride with  
phenylsilanes)

L59 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1978:624407 CAPLUS

DOCUMENT NUMBER: 89:224407

TITLE: The crystal structure of tetrakis(pentafluorophenyl)si  
lane

AUTHOR(S): Karipides, Anastas; Foerst, Barbara

CORPORATE SOURCE: Dep. Chem., Miami Univ., Oxford, OH, USA

SOURCE: Acta Crystallographica, Section B: Structural  
Crystallography and Crystal Chemistry (1978), B34(11),  
3494-6

CODEN: ACBCAR; ISSN: 0567-7408

DOCUMENT TYPE: Journal

LANGUAGE: English

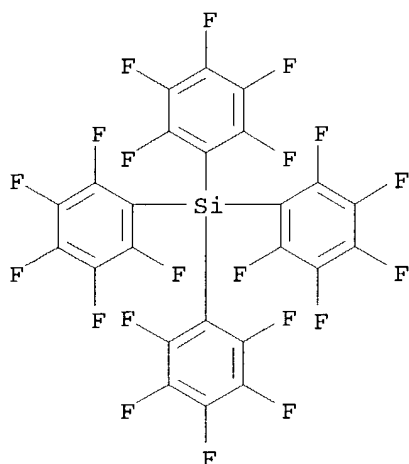
AB The crystal structure of (C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>Si was determined from 3-dimensional  
single-crystal x-ray data collected on a computer-automated  
diffractometer. The compound crystallizes in space group I4<sub>1</sub>/a with cell  
dimensions of a 17.165 (12) and c 8.128 (8) Å; Z = 4. The (C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>Si  
mols. have S<sub>4</sub> crystallog. imposed symmetry. Full-matrix least squares  
refinement yielded a conventional R factor of 0.070.

IT 1524-78-3

RL: PRP (Properties)  
(crystal structure of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 75-5 (Crystallization and Crystal Structure)  
 ST structure pentafluorophenylsilane; fluorophenylsilane structure; silane  
 pentafluorophenyl structure; phenyl pentafluorosilane structure  
 IT Crystal structure  
 Molecular structure  
 (of tetrakis(pentafluorophenyl)silane)  
 IT 1524-78-3  
 RL: PRP (Properties)  
 (crystal structure of)

L59 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:452639 CAPLUS

DOCUMENT NUMBER: 87:52639

TITLE: A fluorine-19 NMR investigation of the transmission of  
 electronic effects in triaryl(4-fluorophenyl)silanes

AUTHOR(S): Pombrik, S. I.; Kravtsov, D. N.; Peregudov, A. S.;  
 Fedin, E. I.; Nesmeyanov, A. N.

CORPORATE SOURCE: Inst. Organo-Elem. Compd., Moscow, USSR

SOURCE: Journal of Organometallic Chemistry (1977), 131(3),  
 355-63

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB For the title compds., a linear relation between the F chemical shifts and  
 the  $\Sigma\sigma_0$  values of the substituted phenyl groups attached to  
 the S atom has been found. The transmission of electronic effects from  
 one aromatic ring to another in tetraarylsilanes occurs mainly by an  
 inductive mechanism. The transmitting ability of Si-C bonds is somewhat  
 higher than that of Sn-C bonds.

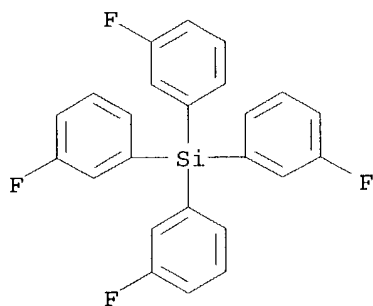
IT 3869-53-2 63523-07-9

RL: PRP (Properties)

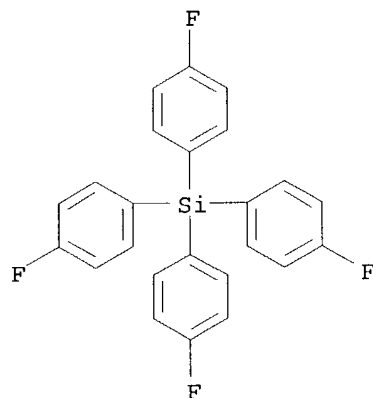
(fluorine-19 NMR spectrum of)

RN 3869-53-2 CAPLUS

CN Silane, tetrakis(3-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 63523-07-9 CAPLUS  
 CN Silane, tetrakis(4-fluorophenyl)- (9CI) (CA INDEX NAME)



CC 22-9 (Physical Organic Chemistry)  
 ST fluorine NMR silane; LFER NMR fluorophenylsilane  
 IT Linear free energy relationship  
 (in fluorine-19 NMR spectra of triaryl(4-fluorophenyl)silanes)  
 IT Nuclear magnetic resonance  
 (of fluorine-19, in triaryl(fluorophenyl)silanes, substituent effect  
 in)  
 IT 3869-53-2 63523-02-4 63523-03-5 63523-04-6 63523-05-7  
 63523-06-8 63523-07-9 63523-08-0 63523-09-1 63523-10-4  
 63523-11-5  
 RL: PRP (Properties)  
 (fluorine-19 NMR spectrum of)  
 IT 349-91-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and reaction of, with trichlorobromobenzene)  
 IT 13190-50-6 21928-51-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with (fluorophenyl)trichlorosilane)



IT 76-86-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with bromofluorobenzene)  
IT 10026-04-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with fluorophenylmagnesium bromide)  
IT 352-13-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with silicon tetrachloride)  
IT 460-00-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with triphenylsilane)

L59 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1973:123476 CAPLUS

DOCUMENT NUMBER: 78:123476

TITLE: NMR studies of pentafluorophenyl-substituted silanes.  
I. Relations between chemical shifts, coupling  
constants, and (p-d) $\pi$  interactions

AUTHOR(S): Haegele, Gerhard; Weidenbruch, Manfred

CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Duesseldorf, Duesseldorf,  
Fed. Rep. Ger.

SOURCE: Chemische Berichte (1973), 106(2), 460-70

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

AB The 60-100 MHz  $^{19}\text{F}$ -NMR spectra of 21 silanes  $\text{R}_n\text{SiX}_{4-n}$  ( $\text{R} = \text{C}_6\text{F}_5$ ,  $n = 1-4$ ,  
 $\text{X} = \text{H}$ , alkyl, halo, or amino),  $\text{RSiMe}_2\text{SiMe}_2\text{R}$ , and  $\text{RSiMe}_2\text{SiMe}_3$  were determined  
and analyzed using [AX]2M approxns. The relations between the title  
parameters were discussed in terms of the  $\pi$ -acceptor action of the  $\text{SiX}$   
groups and long-range interannular F-F and F-H couplings.

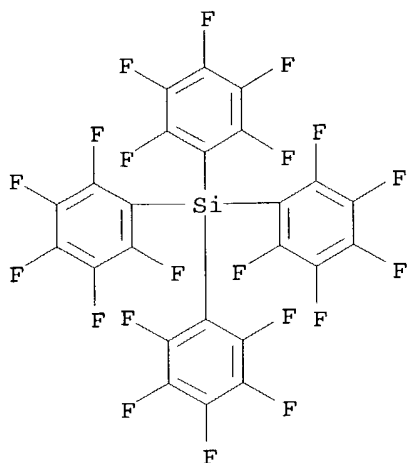
IT 1524-78-3

RL: PRP (Properties)

(NMR of, fluorine-19 of,  $\pi$  interactions in relation to)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



- CC 22-2 (Physical Organic Chemistry)
- ST fluorophenylsilane NMR; silane pentafluorophenyl NMR; fluorine 19 NMR  
fluorophenylsilane; pi acceptor fluorophenylsilane
- IT Conjugation  
(in pentafluorosilanes, NMR in relation to)
- IT Spin, nuclear coupling  
(of fluorine with fluorine, in pentafluorophenylsilanes, conjugation in  
relation to)
- IT Nuclear magnetic resonance  
(of fluorine-19, of pentafluorophenylsilanes, conjugation in relation  
to)
- IT 1206-46-8 1524-78-3 5272-26-4 10536-62-6 17067-70-8  
17067-71-9 18920-98-4 20160-39-8 21655-08-3 27585-17-7  
35369-97-2 35369-98-3 35370-01-5  
RL: PRP (Properties)  
(NMR of, fluorine-19 of,  $\pi$  interactions in relation to)
- IT 7782-41-4, properties  
RL: PRP (Properties)  
(NMR of, in pentafluorophenylsilanes)
- IT 13888-77-2 20160-40-1 23761-73-1 23761-74-2 23761-75-3  
23761-76-4 27490-05-7 27491-93-6 33558-55-3 33558-56-4  
RL: PRP (Properties)  
(NMR of,  $\pi$  interactions in relation to fluorine in)

L59 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1969:119359 CAPLUS

DOCUMENT NUMBER: 70:119359

TITLE: Fragmentation and rearrangement processes in the mass  
spectra of perhalogenoaromatic compounds. II.  
Pentafluorophenyl derivatives of group IV

AUTHOR(S): Miller, Jack M.

CORPORATE SOURCE: Brock Univ., St. Catharines, ON, Can.

SOURCE: Canadian Journal of Chemistry (1969), 47(10), 1613-20  
CODEN: CJCHAG; ISSN: 0008-4042

DOCUMENT TYPE: Journal

LANGUAGE: English

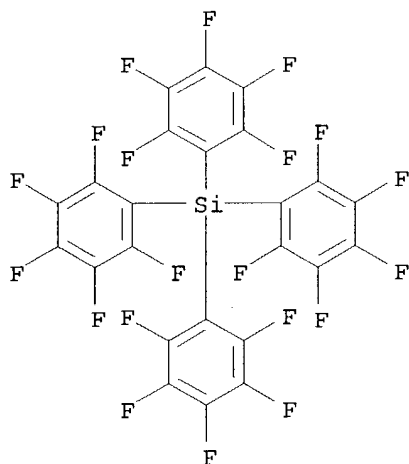
AB The mass spectra of compds. of the type  $(C_6F_5)_4M$  ( $M = Si, Ge, Sn,$  and  $Pb$ ) have been studied. Bond forming rearrangements were detected, involving F abstraction by the central atom, forming perfluorophenylene ions and neutral metal fluoride species. The heavier metals give simpler spectra and fragmentation schemes. The bulk of the ion current is carried by fluorocarbon ions for the Si derivative and by organometallic or metal fluoride ions in the other three cases,  $SnF^+$  and  $PbF^+$  forming the base peaks in their spectra. When  $M$  is C in the compds.  $(C_6F_5)_3COH$  and  $(C_6F_5)_2CO$  there is little evidence for rearrangements and transfer of F to the central C atom.

IT 1524-78-3

RL: PRP (Properties)  
(mass spectrum of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 71 (Electric Phenomena)

ST perhaloaroms mass spectra; silicon perfluorophenyls mass spectra; germanium perfluorophenyls mass spectra; tin perfluorophenyls mass spectra; lead perfluorophenyls mass spectra; perfluorophenyls mass spectra; fluorophenyls mass spectra

IT Mass spectra  
(of Group IVA fluorophenyl derivs.)

IT 1065-49-2 1111-02-0 1452-12-6 1524-78-3

RL: PRP (Properties)  
(mass spectrum of)

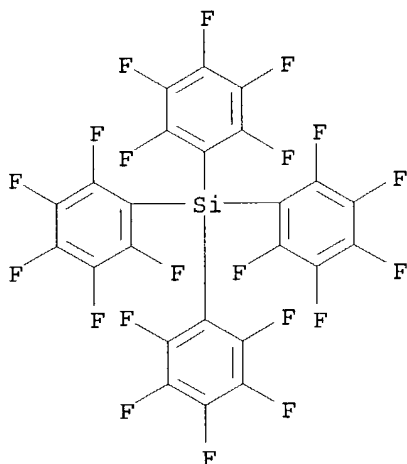
L59 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1968:477334 CAPLUS

DOCUMENT NUMBER: 69:77334

TITLE: A direct preparation of some pentafluorophenyl-containing silanes

AUTHOR(S): Whittingham, A.; Jarvie, A. W. P.  
 CORPORATE SOURCE: Univ. Aston, Birmingham, UK  
 SOURCE: Journal of Organometallic Chemistry (1968), 13(1),  
 125-9  
 CODEN: JORCAI; ISSN: 0022-328X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The reaction of pentafluorobromobenzene with both tetraethoxysilane and  
 tetrachlorosilane, by a modified Grignard method, leads to the formation  
 of compds. of the type (C<sub>6</sub>F<sub>5</sub>)<sub>n</sub>SiX<sub>4-n</sub> (X = OEt and Cl and n = 1 - 4).  
 These compds. have been characterized by phys. methods, elemental anal.,  
 interconversion and the preparation of derivs.  
 IT **1524-78-3P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 1524-78-3 CAPLUS  
 CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)  
 ST silanes perfluorophenyl; silicon org compds  
 IT 1206-46-8P **1524-78-3P** 10536-62-6P 13888-69-2P 20083-34-5P  
 20083-38-9P 20160-45-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

L59 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1968:456104 CAPLUS  
 DOCUMENT NUMBER: 69:56104  
 TITLE: The fluorine-19 NMR spectra of some pentafluorophenyl  
 compounds of group IV elements  
 AUTHOR(S): Jolley, K. W.; Sutcliffe, L. H.  
 CORPORATE SOURCE: Univ. Liverpool, Liverpool, UK  
 SOURCE: Spectrochimica Acta, Part A: Molecular and  
 Biomolecular Spectroscopy (1968), 24(8), 1191-203

CODEN: SAMCAS; ISSN: 1386-1425

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Accurate chemical shifts were determined for the pentafluorophenyl F nuclei of  
a

number of Group IV pentafluorophenyl compds. by the use of an extended lock in the HA mode. All the compds. studied have a very large ortho shift, the trends of which can be predicted by both the van der Waals elec. field theory and the through bond theory of Hruska, et al. The m- and p-<sup>19</sup>F chemical shifts were used to predict the  $\pi$ -electron accepting ability of the various substituents attached to the Group IV atom. The coupling consts. obtained from those compds. which give resolvable spectra supports the chemical shift work. 35 references.

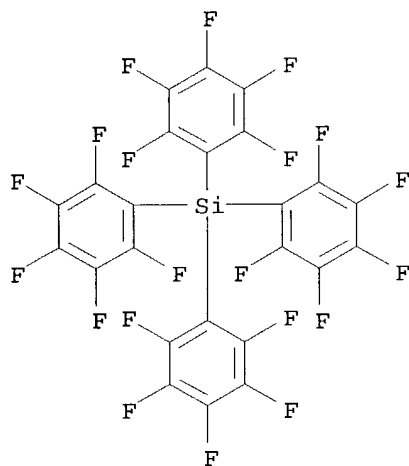
IT 1524-78-3

RL: PRP (Properties)

(nuclear magnetic resonance of fluorine in)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 73 (Spectra and Other Optical Properties)

ST NMR F 19 fluorophenyls; fluorine 19 NMR; fluorophenyls NMR

IT Substituents

(electron accepting ability of, of Group IV compds., N.M.R. in determination of)

IT Electron acceptors

(nuclear magnetic resonance in determination of)

IT Nuclear magnetic resonance

(of fluorine, in (pentafluorophenyl) derivs. of Group IV elements)

IT 801-79-6 1015-53-8 1058-08-8 1062-67-5 1062-71-1 1065-49-2  
1080-51-9 1106-04-3 1111-02-0 1259-89-8 1262-57-3 1452-12-6  
1524-78-3 10177-67-0 10177-68-1 10177-69-2 10360-39-1

RL: PRP (Properties)

(nuclear magnetic resonance of fluorine in)

L59 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1968:13065 CAPLUS

DOCUMENT NUMBER: 68:13065

TITLE: Polyhalo-organometallic and -organometalloidal compounds. VIII. Preparation of some pentafluorophenyl substituted organosilicon compounds

AUTHOR(S): Fearon, F. W. Gordon; Gilman, Henry

CORPORATE SOURCE: Iowa State Univ., Ames, IA, USA

SOURCE: Journal of Organometallic Chemistry (1967), 10(3), 409-19

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal

LANGUAGE: English

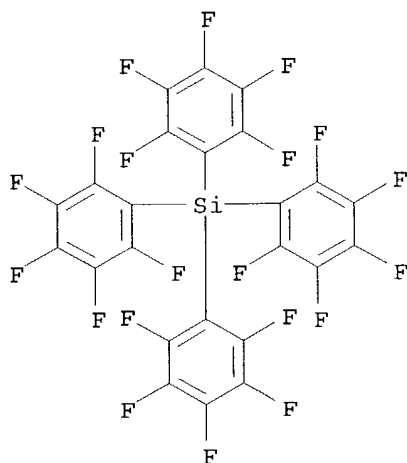
AB The preparation and some properties of  $(C_6F_5)_nSiPh_{4-n}$  (where  $n = 1-4$ ) and  $(C_6F_5)_nPh_{3-n}SiX$  (where  $n = 1$  or  $2$  and  $X = H$  or  $Cl$ ) are described. In general, these compds. were obtained by the reaction of a (pentafluorophenyl)metallic compound with the corresponding chlorosilane. However,  $(C_6F_5)_nPh_{3-n}SiCl$  could not be obtained in this manner; they were prepared by the chlorination of the corresponding organosilicon hydrides. Evidence is presented which suggests that  $C_6Cl_5Li$  is more reactive towards  $ClSiPh_3$  than is  $C_6F_5Li$  under similar conditions. The reaction of an alkyl lithium compound with  $HPh_2SiC_6F_5$  leads predominantly to cleavage of the  $C_6F_5$  group from  $Si$ . The ir spectra of all the above compds. are discussed and the uv spectra of  $(C_6F_5)_nSiPh_{4-n}$  (where  $n = 1-4$ ) are reported. 18 references.

IT 1524-78-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)

ST SILANES PENTAFLUOROPHENYL; FLUORO AROM SILANES

IT 1206-46-8P 1524-78-3P 17067-69-5P 17067-70-8P 17067-71-9P

17067-73-1P 17067-74-2P 17067-75-3P 17067-76-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

L59 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1965:498496 CAPLUS

DOCUMENT NUMBER: 63:98496

ORIGINAL REFERENCE NO.: 63:18136a-b

TITLE: Pentafluorophenyl organometallic compounds of group IV elements

AUTHOR(S): Tamborski, C.; Soloski, E. J.; Dec, S. M.

CORPORATE SOURCE: Wright Patterson Air Force Base, Dayton, OH

SOURCE: Journal of Organometallic Chemistry (1965), 4(6), 446-54

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal

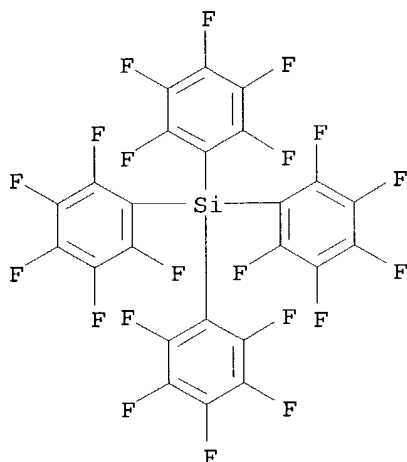
LANGUAGE: English

AB The synthesis of pentafluorophenyl group IV elements (C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>Si, (C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>Ge, (C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>Sn, (C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>Pb, (C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>Ti (C<sub>5</sub>F<sub>5</sub>)<sub>2</sub> and (C<sub>6</sub>H<sub>5</sub>)<sub>2</sub>Zr(C<sub>6</sub>F<sub>5</sub>)<sub>2</sub> is reported. The above compounds are prepared through the reaction of the appropriate metal halide and pentafluorophenyllithium. The various pentafluorophenyl derivatives are subjected to the following studies: infrared and vapor phase chromatography analysis, acid and base hydrolysis, thermal stability, and reactions with bromine and lithium.

IT 1524-78-3, Silane, tetrakis(pentafluorophenyl)-  
(preparation of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 39 (Organometallic and Organometalloidal Compounds)

IT Organometallic compounds  
(heterocyclic)

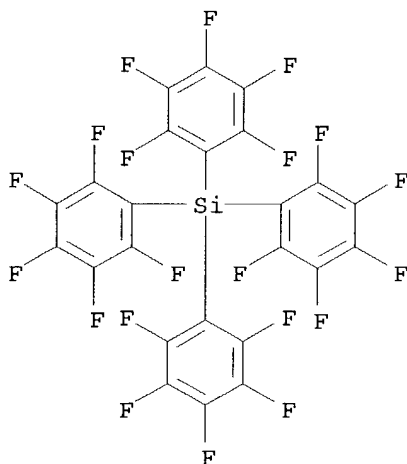
IT Heterocyclic compounds  
(metal complexes)

IT Spectra, infrared  
 (of tetrakis(pentafluorophenyl) derivs. of Group IV elements)  
 IT 1065-49-2, Tin, tetrakis(pentafluorophenyl)- 1111-02-0, Lead,  
 tetrakis(pentafluorophenyl)- 1452-12-6, Germane,  
 tetrakis(pentafluorophenyl) 1524-78-3, Silane,  
 tetrakis(pentafluorophenyl)- 12097-97-1, Zirconium,  
 dicyclopentadienylbis(pentafluorophenyl)- 12155-89-4, Titanium,  
 dicyclopentadienylbis(pentafluorophenyl)-  
 (preparation of)

L59 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1964:17001 CAPLUS  
 DOCUMENT NUMBER: 60:17001  
 ORIGINAL REFERENCE NO.: 60:3009f-g  
 TITLE: Tetrakis(pentafluorophenyl)silane  
 INVENTOR(S): Pummer, Walter J.; Wall, Leo A.  
 PATENT ASSIGNEE(S): United States Dept. of the Navy  
 SOURCE: 1 p.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
	US 3109855		19631105	US	19610626
AB	Division of U.S. 3,046,313 (CA 57, 15003a). Pentafluorobromobenzene (I) is converted to the Grignard reagent and the Grignard reagent is treated with SiCl <sub>4</sub> to give the title compound, which can be used as a fuel-resistant substance. I (24.7 g.) and a small crystal of iodine are added to a mixture of 2.4 g. Mg in 50 ml. anhydrous ether, the mixture cooled to 0°, 2.83 ml. SiCl <sub>4</sub> added, the mixture agitated 1 hr. at 0°, refluxed 2.5 hrs., and allowed to cool overnight. The mixture is poured into 100 ml. 6N HCl, and the precipitate obtained separated, dried, and sublimed at 208° at 1 mm. to give 5.5 g. tetrakis(pentafluorophenyl)silane, m. 246-8°, 32% yield.				
IT	1524-78-3, Silane, tetrakis(pentafluorophenyl)- (preparation of)				
RN	1524-78-3 CAPLUS				
CN	Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)				





NCL 260448200  
 CC 39 (Organometallic and Organometalloidal Compounds)  
 IT 1524-78-3, Silane, tetrakis(pentafluorophenyl)-  
 (preparation of)

L59 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1962:475681 CAPLUS  
 DOCUMENT NUMBER: 57:75681  
 ORIGINAL REFERENCE NO.: 57:15003a-f  
 TITLE: Pentafluoriodobenzene  
 INVENTOR(S): Pummer, Walter J.; Wall, Leo A.  
 PATENT ASSIGNEE(S): U.S. Dept. of the Navy  
 SOURCE: 3 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3046313		19620724	US	19600503

AB Pentafluoriodobenzene (I), an intermediate in the preparation of perfluorophenyl derivs., was prepared from pentafluorobromobenzene (II) via the Grignard reagent or by iodination of pentafluorobenzene (III). Thus, to a refluxing solution of the Grignard reagent from 10 g. II and 1 g. Mg in 10 ml. Et<sub>2</sub>O was added 9.76 g. F<sub>2</sub>ClCCHFI in 5 ml. Et<sub>2</sub>O, the mixture refluxed 3 hrs., let stand overnight, 50 ml. 6N HCl added, the Et<sub>2</sub>O layer separated, dried, and distilled to give 5.78 g. I, b<sub>35</sub> 77-8°, n<sub>20D</sub> 1.4990. In another example the same amount of Grignard-reagent solution was treated at 0° with 12.4 g. F<sub>2</sub>C:CFI, the mixture stirred 1 hr., refluxed 2 hrs., and worked up as before to yield 1 g. I. I was also prepared by adding 255 g. mixture of 45% hexafluorobenzene, 40% III, and 10% tetrafluorobenzene to 200 g. iodine in 1 kg. 65% oleum. The mixture was stirred 4 hrs. at 55-60°, let cool overnight, then in an ice bath, diluted with 2 l. ice H<sub>2</sub>O, decolorized with aqueous NaHSO<sub>3</sub>, and separated The crude I (177 g.) was

dried and distilled to give 36 g. I. Condensation of II in the presence of Cu powder at 180-90° 48 hrs. then at 290° 6 hrs. gave 87% (C<sub>6</sub>F<sub>5</sub>)<sub>2</sub>, sublimed at 50°/1 mm., m. 67.5-68°. I (5 g.) and 1.6 g. CuCN heated to 150° in 1.34 g. C<sub>5</sub>H<sub>5</sub>N, cooled to 100°, and distilled gave 3.07 g. crude C<sub>6</sub>F<sub>5</sub>CN (IV), b. 185-90°, n<sub>D</sub><sup>20</sup> 1.4764. Hydrolysis of IV with 75% H<sub>2</sub>SO<sub>4</sub> at 180° gave 16% C<sub>6</sub>F<sub>5</sub>CO<sub>2</sub>H, m. 101-3°. To the Grignard reagent from 10 g. II was added 6.6 g. AcH at 0°, the solution stirred 1 hr. at 0°, decomposed with 50 ml. 6N HCl, the Et<sub>2</sub>O layer separated, dried, and distilled to give 81%

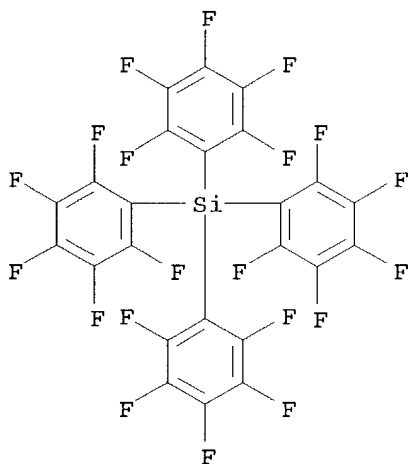
C<sub>6</sub>F<sub>5</sub>CHMeOH

(V), b<sub>37</sub> 80-2°, n<sub>D</sub><sup>20</sup> 1.4426. To the Grignard reagent from 24.7 g. II in 50 ml. Et<sub>2</sub>O was added 4.25 g. SiCl<sub>4</sub> at 0°, the mixture stirred 0.5 hr. at 0° refluxed 2.5 hrs., let cool overnight, poured into 100 ml. 6N HCl, and filtered. The solid was sublimed at 208°/1 mm. to give 32% (C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>Si, m. 246-8°. To the Grignard reagent from 30 g. II in 0.75 ml. Et<sub>2</sub>O was added 5.0 g. PCl<sub>3</sub> in 20 ml. Et<sub>2</sub>O in an ice bath, the mixture let stand at room temperature 15 min., hydrolyzed with 40 ml. cold 10% HCl, the Et<sub>2</sub>O layer separated, dried, and concentrated Sublimation at 100-30° under reduced pressure gave 39.5% (C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>P (VI), m. 114-15°. Oxidation of 2.0 g. VI by refluxing in 10 g. Na<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>, 25 ml. H<sub>2</sub>O, 10 ml. concentrated H<sub>2</sub>SO<sub>4</sub>, and 25 ml. AcOH gave, after neutralization and extraction with CHCl<sub>3</sub>, 2 g. (C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>PO, m. 167-8°. Pyrolysis of 2 g. V over Al<sub>2</sub>O<sub>3</sub> at 345-50° gave, after distillation, 0.6 g. C<sub>6</sub>F<sub>5</sub>CH:CH<sub>2</sub>, b. 140-1°, n<sub>D</sub><sup>20</sup> 1.4414.

IT 1524-78-3, Silane, tetrakis(pentafluorophenyl)-  
(preparation of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 29 (Noncondensed Aromatic Compounds)

IT Benzene, tetrabromo-  
(manufacture of)

IT 608-71-9, Phenol, pentabromo-  
(manufacture of)

IT 87-82-1, Benzene, hexabromo- 108-72-5, 1,3,5-Benzenetriamine 434-90-2,  
 Biphenyl, decafluoro- 602-94-8, Benzoic acid, pentafluoro- 653-34-9,  
 Styrene, 2,3,4,5,6-pentafluoro- 773-82-0, Benzonitrile, pentafluoro-  
 827-15-6, Benzene, pentafluoroiodo- 830-50-2, Benzyl alcohol,  
 2,3,4,5,6-pentafluoro- $\alpha$ -methyl- 1259-35-4, Phosphine,  
 tris(pentafluorophenyl)- 1524-78-3, Silane,  
 tetrakis(pentafluorophenyl)- 2729-11-5, Phosphine oxide,  
 tris(pentafluorophenyl)- 13654-09-6, Biphenyl, decabromo- 27858-07-7,  
 Biphenyl, octabromo- 90823-46-4, Aniline, tetrabromo-  
 (preparation of)

L59 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1962:429701 CAPLUS

DOCUMENT NUMBER: 57:29701

ORIGINAL REFERENCE NO.: 57:5944a-h

TITLE: Synthesis of organosilicon compounds, particularly  
 those containing halophenyl groups

AUTHOR(S): Gilman, Henry; Gorsich, Richard D.; Gaj, Bernard J.

CORPORATE SOURCE: Iowa State Univ., Ames

SOURCE: Journal of Organic Chemistry (1962), 27, 1023-6  
 CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. CA 55, 5416e. Tetrasubstituted silanes  $R_nSiR'_4-n$  (I) were prepared by  
 treating  $RLi$  with the appropriate chlorosilane or  $SiCl_4$ . Several compds.,  
 $R_3SiR'SiR_3$  (II) were prepared  $BuLi$  (0.05 mole) in 170 ml.  $Et_2O$  stirred  
 rapidly with gradual addition of 0.05 mole  $m-C_6H_4BrF$  in 95 ml.  $Et_2O$  at  
 $-45^\circ$ , the mixture stirred 20 min. at  $-40^\circ$  and carbonated, the  
 organic layer extracted with  $NaHCO_3$ , the extract boiled and acidified with  
 concentrated

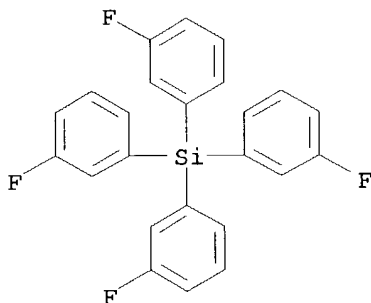
$HCl$  yielded 65%  $m-FC_6H_4CO_2H$ , m.  $123-4^\circ$ .  $Cl_2SiPh_2$  (0.05 mole) in 80  
 ml.  $Et_2O$  stirred with gradual addition of 0.12 mole  $m-FC_6H_4Li$  in 200 ml.  $Et_2O$   
 and the mixture stirred 8 hrs. at  $20^\circ$ , refluxed 2 hrs. and the  
 product taken up in ligroine (b.  $60-70^\circ$ ), the solution decolorized  
 (Norit) and evaporated yielded 26% I ( $R = m-FC_6H_4$ ,  $R' = Ph$ ,  $n = 2$ ), m.  
 $195-6^\circ$ . Similarly were prepared I ( $R = m-FC_6H_4$ ) ( $R'$ , n, m.p. or  
 b.p./mm., and % yield given): Ph, 1,  $207-8^\circ$  (AcOH), 51; Ph, 2,  
 $195-6^\circ$  (ligroine), 26; Ph, 3,  $191.5-3.0^\circ$  (dioxane), 51; 0,  
 $4$ ,  $196-7^\circ$  (ligroine), 62;  $Cl_2H_25$ , 3,  $35-7^\circ$ , 197  
 $8^\circ/0.02$ ,  $n_{25D}$  1.5358, 62;  $Cl_6H_{33}$ , 8,  $36-8^\circ$ ,  
 $214-17^\circ/0.05$ , 71;  $Cl_8H_{37}$ , 3,  $38-40^\circ$ ,  $234-5^\circ/0.08$ , 71.  
 $GeCl_4$  (8.0 g.) and 0.178 mole  $m-FC_6H_4Li$  in 300 ml.  $Et_2O$  yielded 25%  
 $(m-FC_6H_4)_4Ge$ , m.  $194-5^\circ$  (ligroine). Similarly were prepared I using  
 $m-ClC_6H_4Li$  or  $p-ClC_6H_4Li$  ( $R$ ,  $R'$ , n, m.p. or b.p./mm.,  $n_{25D}$ ,  $d_{25}$ , MR, and %  
 yield given):  $m-ClC_6H_4$ , Ph, 1,  $156-7^\circ$  (alc.), 78;  $m-ClC_6H_4$ , Ph, 2,  
 $110-11^\circ$  (alc.), 80;  $m-ClC_6H_4$ , Ph, 3,  $87.5-9.0^\circ$  (alc.), 43;  
 $m-ClC_6H_4$ , -, 4,  $148-9^\circ$  (ligroine), 43;  $m-ClC_6H_4$ ,  $Cl_2H_25$ , 3,  
 $229-30^\circ/0.086$  -, -, -, 78.5;  $m-ClC_6H_4$ ,  $Cl_6H_{33}$ , 3,  
 $240-1^\circ$ /less than 0.01, 1.5579, 1.078, 175.9, 65.8;  $m-ClC_6H_4$ ,  
 $Cl_2H_25$ , 3,  $250-5^\circ/0.04$ , 1.5595, 1.085, 183.5, 87.4;  $p-ClC_6H_4$ ,  
 $Cl_6H_{33}$ , 3,  $246-51^\circ/0.03$ , 1.5530, 1.071, 175.7, 65.6;  $p-ClC_6H_4$ ,  
 $Cl_8H_{37}$ , 3,  $255-62^\circ/0.001$ , 1.5558, 1.075, 183.4, 76.8.  $PhCH_2MgCl$

(25.3 g. PhCH<sub>2</sub>Cl, 4.86 g. Mg) in 200 ml. Et<sub>2</sub>O added with stirring to 5.9 g. Cl<sub>3</sub>SiCH<sub>2</sub>CH<sub>2</sub>SiCl<sub>3</sub> in 55 ml. Et<sub>2</sub>O and the mixture distilled 12 hrs., the Et<sub>2</sub>O replaced with xylene and refluxed 50 hrs. at 100°, hydrolyzed with 5% HCl and the product (11.6 g.) recrystd. 3 times from ligroine (b. 60-70°) and from EtOAc yielded 81% II [R = PhCH<sub>2</sub>, R' = (CH<sub>2</sub>)<sub>2</sub>], m. 136-7°. Similarly were prepared II (R, R', m.p. or b.p./mm., and % yield given): BuCH(Et)CH<sub>2</sub>, (CH<sub>2</sub>)<sub>2</sub>, 215-20°/0.04, 54; Cl<sub>6</sub>H<sub>3</sub>, (CH<sub>2</sub>)<sub>2</sub>, 43-5° (CCl<sub>4</sub>-alc.), 75; PhCH<sub>2</sub>, m-C<sub>6</sub>H<sub>4</sub>, 155-7° (EtOAc), 16; Cl<sub>10</sub>H<sub>21</sub>, m-C<sub>6</sub>H<sub>4</sub>, 285-8°/0.03, n<sub>20</sub>D 1.4811, d<sub>20</sub> 0.863, MR 323.8, 58; Cl<sub>10</sub>H<sub>21</sub>, p-C<sub>6</sub>H<sub>4</sub>, 290-4°/0.07, 20. Li (0.9 g.) in 60 ml. Et<sub>2</sub>O and 8.0 g. BrCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH:CH<sub>2</sub> in 70 ml. Et<sub>2</sub>O at -30° treated with 7.38 g. Ph<sub>3</sub>SiCl in 60 ml. Et<sub>2</sub>O and the mixture stirred 15 min. at 0° and 11 hrs. at 20°, hydrolyzed and the product distilled in vacuo gave material, b<sub>0.15</sub> 155-7°, recrystd. from alc. (ice bath) to yield 67% H<sub>2</sub>C:CH(CH<sub>2</sub>)<sub>3</sub>SiPh<sub>3</sub> (III), m. 45-6°. Ph<sub>3</sub>SiH (26 g.), 3.4 g. III, and 0.32 g. Bz<sub>2</sub>O<sub>2</sub> stirred 20 hrs. at 80° in 25 ml. C<sub>6</sub>H<sub>14</sub> and freed from excess Ph<sub>3</sub>SiH at 148-60°/0.7 mm., the gummy solid crystallized from alc.MeCOEt and the product, m. 140-3°, recrystd. from alc.-EtOAc yielded 65% pure II [R = Ph, R' = (CH<sub>2</sub>)<sub>5</sub>] (IV), m. 145-6°. Li(CH<sub>2</sub>)<sub>5</sub>Li (from 20 g. Br(CH<sub>2</sub>)<sub>5</sub>Br) in 180 ml. Et<sub>2</sub>O treated at -20° with 17.4 g. Ph<sub>3</sub>SiCl in 160 ml. Et<sub>2</sub>O and the mixture stirred 16 hrs. at 20°, hydrolyzed and the product crystallized from EtOAc gave IV. Et<sub>2</sub>O (30 ml.) containing 6 g. (3-BrC<sub>6</sub>H<sub>4</sub>)<sub>2</sub> added with stirring to 0.038 mole BuLi in 75 ml. Et<sub>2</sub>O at -30° and the mixture stirred 6 hrs. at 20°, refluxed 15 min. and the insol. reagent refluxed 45 min. with 11.3 g. Ph<sub>3</sub>SiCl in 100 ml. Et<sub>2</sub>O, diluted with 100 ml. C<sub>6</sub>H<sub>6</sub> and distilled to a pot temperature of 53°, refluxed 15 min. and hydrolyzed, the mixture filtered and the product recrystd. from H<sub>2</sub>O-dioxane yielded 69% II (R = Ph, R' = 3,3'-biphenylene), m. 221-3°.

IT 3869-53-2, Silane, tetrakis(m-fluorophenyl)-  
(preparation of)

RN 3869-53-2 CAPLUS

CN Silane, tetrakis(3-fluorophenyl)- (9CI) (CA INDEX NAME)



CC 33 (Organometallic and Organometalloidal Compounds)

IT 7803-62-5, Silane  
(halophenyl derivs.)

IT 2128-45-2, Silane, dodecyltris(m-fluorophenyl)- 2376-83-2, Silane,  
tris(m-fluorophenyl)hexadecyl- 2559-39-9, Silane, (m-

fluorophenyl)triphenyl- 2736-28-9, Silane, 4-pentenyltriphenyl-  
 2794-05-0, Silane, tris(m-fluorophenyl)octadecyl- 2804-88-8, Silane,  
 tris(m-fluorophenyl)phenyl- 2804-94-6, Silane, bis(m-  
 fluorophenyl)diphenyl- 3797-46-4, Germane, tetrakis(m-fluorophenyl)  
**3869-53-2**, Silane, tetrakis(m-fluorophenyl)- 18733-70-5, Silane,  
 bis(m-chlorophenyl)diphenyl- 18733-82-9, Silane, tetrakis(m-  
 chlorophenyl)- 18733-90-9, Silane, tris(m-chlorophenyl)phenyl-  
 18737-43-4, Silane, (m-chlorophenyl)triphenyl- 18759-06-3, Silane,  
 tris(m-chlorophenyl)hexadecyl- 18759-07-4, Silane, tris(p-  
 chlorophenyl)hexadecyl- 18764-96-0, Silane, tris(m-chlorophenyl)dodecyl-  
 18817-52-2, Silane, tris(m-chlorophenyl)octadecyl- 18817-86-2, Silane,  
 tris(p-chlorophenyl)octadecyl- 18826-15-8, Silane, 3,3'-  
 biphenyllylenebis[triphenyl- 18828-71-2, 2,5-Disilaheptane,  
 2,2,5,5-tetrabenzyl-1,6-diphenyl- 18840-86-3, Silane,  
 m-phenylenebis[tribenzyl- 18846-53-2, 1,7-Disilaheptane,  
 1,1,1,7,7,7-hexaphenyl- 18863-01-9, Silane, m-phenylenebis[trisdecyl]-  
 18863-02-0, Silane, p-phenylenebis[tris(decyl)- 18867-29-3,  
 17,20-Disilaheptatriacontane, 17,17,20,20-tetrahexadecyl- 18870-57-0,  
 Benzhydrol,  $\alpha$ -[(methyldiphenylsilyl)methyl]- 18882-14-9,  
 7,10-Disilaheptadecane, 5,12-diethyl-7,7,10,10-tetrakis(2-ethylhexyl)-  
 (preparation of)

L59 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1961:93280 CAPLUS

DOCUMENT NUMBER: 55:93280

ORIGINAL REFERENCE NO.: 55:17557a-c

TITLE: Preparation and thermal stability of  
 tetrakis(pentafluorophenyl)silane and  
 tris(pentafluorophenyl)phosphine

AUTHOR(S): Wall, Leo A.; Donadio, Robert E.; Pummer, Walter J.

CORPORATE SOURCE: Natl. Bur. of Standards, Washington, DC

SOURCE: Journal of the American Chemical Society (1960), 82,  
 2846-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

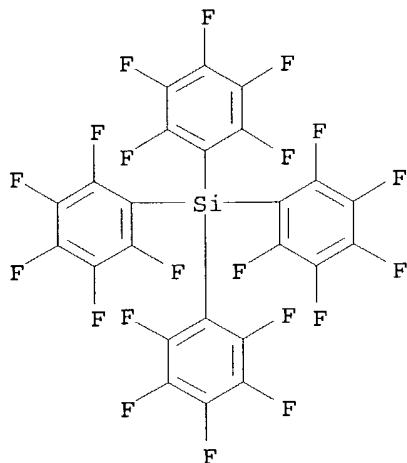
LANGUAGE: Unavailable

AB To  $C_6F_5MgBr$  (from 24.7 g.  $C_6F_5Br$ , 2.43 g. Mg and 50 ml. dry  $Et_2O$ ) was  
 added dropwise 4.25 g.  $SiCl_4$  at  $0^\circ$ , the whole stirred 1 hr. at  
 $0^\circ$  and refluxed 3 hrs. to give 32%  $(C_6F_5)_4Si$  (I), m.  $248-50^\circ$   
 (sublimation at  $208^\circ/1$  mm. followed by recrystn. from  $Me_2CO-C_6H_6$ ),  
 $\lambda$  6.57, 7.72, 9.1, 10.26  $\mu$ . Attempts to prepare  $(C_6F_5)_2SiCl_2$  by  
 this procedure gave some I and tars. The same procedure gave 39.5%  
 $(C_6F_5)_3P$  (II), m.  $116-17^\circ$ ,  $\lambda$  6.08, 6.57, 6.78, 10.25  $\mu$ ,  
 $\lambda_{MeOHmax}$ . 253  $m\mu$  ( $\epsilon = 10,400$ ). II (2.0 g.), 10 g.  
 $Na_2CrO_7$ , 25 ml.  $H_2O$ , 10 ml. concentrated  $H_2SO_4$ , and 25 ml.  $AcOH$  refluxed 6 hrs.  
 gave 2.0 g.  $(C_6F_5)_3PO$  (III), m.  $169-70^\circ$  (petr. ether),  $\lambda$   
 6.08, 6.59, 6.75, 8.15, 10.15  $\mu$ ;  $\lambda_{MeOHmax}$ . 2.75, 250  $m\mu$   
 ( $\epsilon = 2600, 730$ ). The thermal stability of I, II, III,  $Ph_2$  (IV),  
 $(C_6F_5)_2$  (V),  $Ph_4Si$  (VI), and  $Ph_3P$  (VII) at  $200-660^\circ$  indicated the  
 following order:  $V \geq IV > VI \geq I > II > VII > III$ .

IT 1524-78-3, Silane, tetrakis(pentafluorophenyl)-  
 (preparation and thermal stability of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 10E (Organic Chemistry: Benzene Derivatives)

IT Phosphine, diphenylpiperidino-

IT 1259-35-4, Phosphine, tris(pentafluorophenyl)- 1524-78-3,  
Silane, tetrakis(pentafluorophenyl)- 2729-11-5, Phosphine oxide,  
tris(pentafluorophenyl)-

(preparation and thermal stability of)

IT 35259-94-0, Phosphine sulfide, diphenylpiperidino-  
(preparation of)

IT 92-52-4, Biphenyl 434-90-2, Biphenyl, decafluoro- 603-35-0, Phosphine,  
triphenyl- 1048-08-4, Silane, tetraphenyl-  
(thermal stability of)

=>